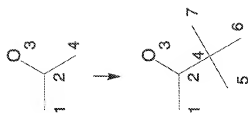
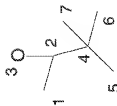


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Resultant molecule



...and the molecule it represents

Atom Elm Bonded To

1	C	2
2	C	1,3,4
3	O	2
4	C	2,5,6,7
5	C	4
6	C	4
7	C	4

Simplified
Connection Table

FIG. 1A

(Prior Art)

FIG. 1B

(Prior Art)

FIG. 1C

Two different ring
systems are present

Spiro



Fused



Bridged

FIG. 2

(Prior Art)

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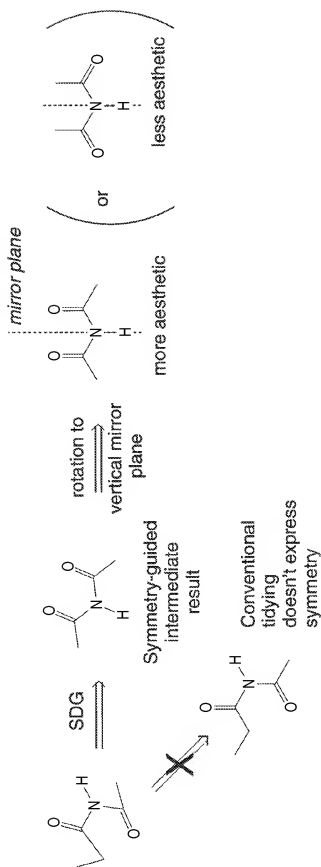


FIG. 3

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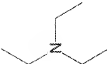
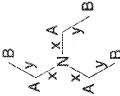




	<p>a. Given structure (Starting coordinates are irrelevant.)</p>		<p>b. Perceived symmetry. Like letters indicate equivalent atoms or bonds. Symmetry is three-fold.</p>	N	<p>c. The pivot atom is taken as the first seed atom.</p>		<p>d. Place an adjacent atom.</p>
	<p>e. Place equivalent atoms, with three- fold symmetry</p>		<p>f. Place next atom. (Direction is arbitrary.)</p>		<p>g. Place equivalent atoms, with three- fold symmetry.</p>		

FIG. 4

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	<p>a. Given structure (Starting coordinates are irrelevant.)</p>		<p>b. Perceived symmetry. Like letters indicate equivalent atoms. Symmetry is reflection.</p>		<p>d. Because it is cyclic, we deposit the whole ring as one unit.</p>		<p>e. Place next atom.</p>
	<p>f. Place equivalent atom, with reflectional symmetry</p>		<p>g. Place next atom. (Direction is arbitrary.)</p>		<p>h. Place equivalent atom, with reflectional symmetry.</p>		<p>i. Place next atom.</p>
	<p>j. Place equivalent atom, with reflectional symmetry.</p>						

FIG. 5

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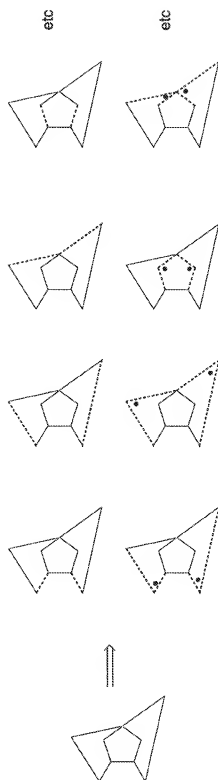


FIG. 6

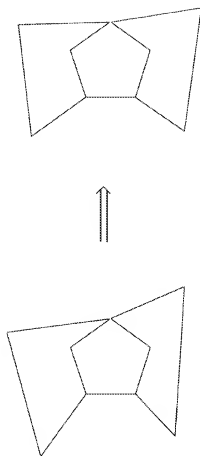
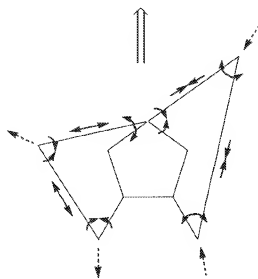


FIG. 7



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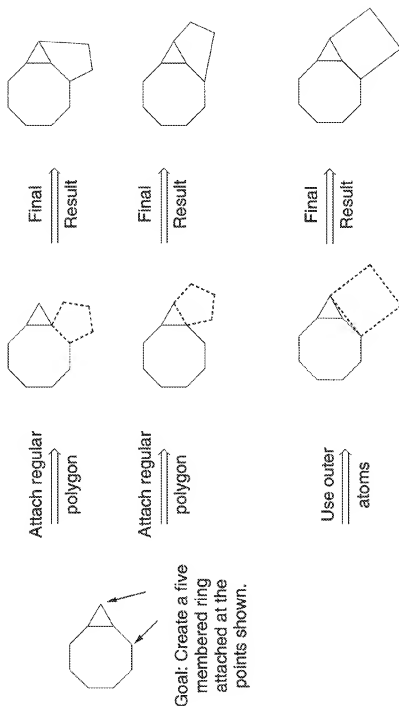


FIG. 8

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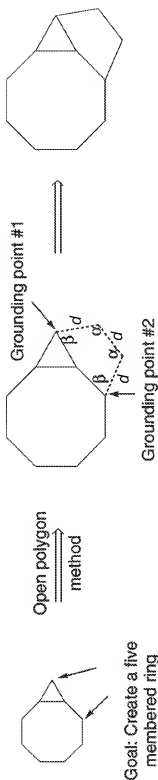
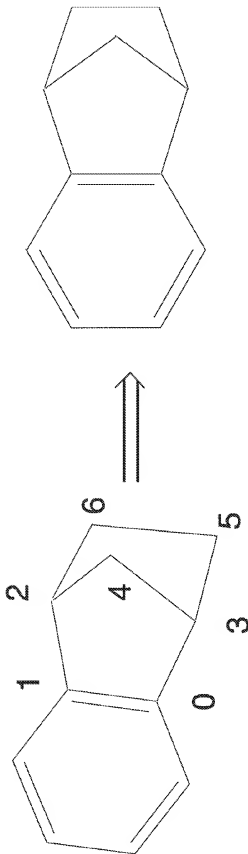


FIG. 9



FIG. 10



-----Enter RD_AttachPeeledBridge [3]

Attaching peeled bridge at atoms 2 (CW) and 3 (CCW)

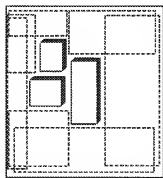
```
Rating for bd len scale 1.0 is 198.294 (= congest[ 178.294] + BdLen[0.00] + bdAng[ 20 (bdAng=125)])
Rating for bd len scale 0.5 is 313.185 (= congest[ 45.185] + BdLen[40.00] + bdAng[228 (bdAng=177)])
Rating for bd len scale 0.7 is 291.643 (= congest[ 179.643] + BdLen[24.00] + bdAng[ 88 (bdAng=142)])
Rating for bd len scale 0.9 is 242.107 (= congest[ 178.107] + BdLen[8.00] + bdAng[ 56 (bdAng=134)])
Rating for bd len scale 1.1 is 93.917 (= congest[ 85.917] + BdLen[8.00] + bdAng[ 0 (bdAng=119)])
Rating for bd len scale 1.3 is 56.154 (= congest[ 32.154] + BdLen[24.00] + bdAng[ 0 (bdAng=109)])
Rating for bd len scale 1.5 is 61.044 (= congest[ 21.044] + BdLen[40.00] + bdAng[ 0 (bdAng=103)])
Rating for bd len scale 1.7 is 72.576 (= congest[ 16.576] + BdLen[56.00] + bdAng[ 0 (bdAng=98)])
Rating for bd len scale 1.9 is 86.400 (= congest[ 14.400] + BdLen[72.00] + bdAng[ 0 (bdAng=94)])
```

Ring 1: Best bridge scale factor = 1.30 (rating = 56.154)

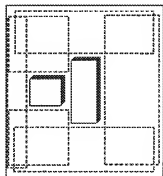
Irregular polygon. (numAtsToDraw=4; RINGSIZ=5; aOuter_CW=2; _CCW=3)

-----Exit RD_AttachPeeledBridge

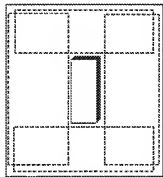
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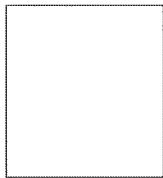
d. After imprinting the third box, there are eight free rectangles. (Translation step not included for clarity.)



c. After imprinting the second box, there are seven free rectangles. (Translation step not included for clarity.)



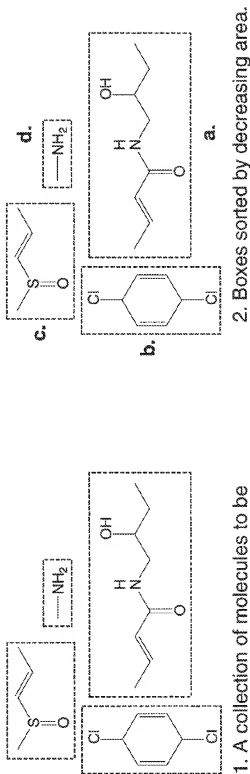
b. After imprinting the first box, there are four free rectangles.



a. Initial free rectangle

FIG. 12

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1. A collection of molecules to be positioned, with their enclosing boxes.

2. Boxes sorted by decreasing area.

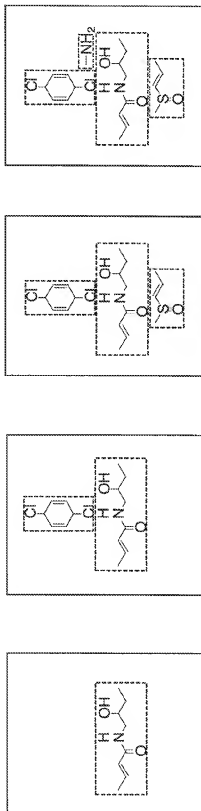


FIG. 13

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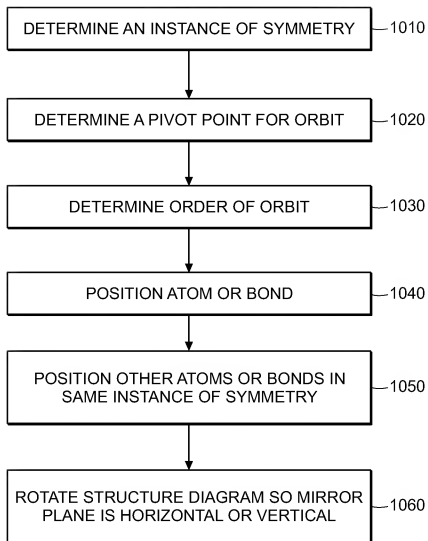


FIG. 14

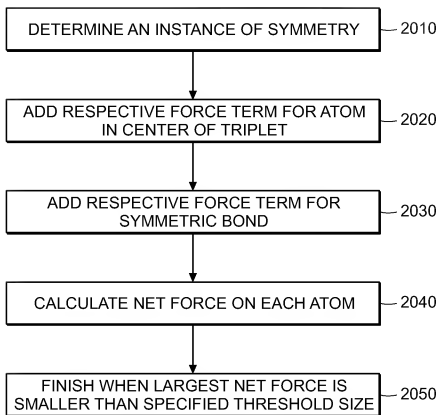


FIG. 15

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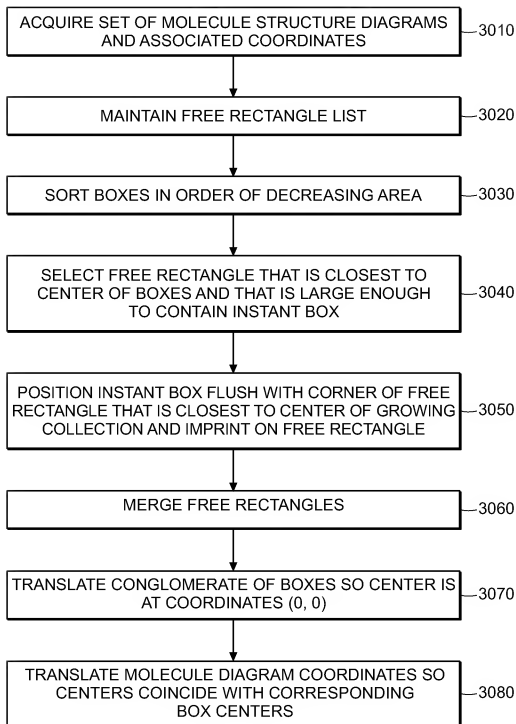


FIG. 16